10-423/10-623 Generative AI

Machine Learning Department
School of Computer Science
Carnegie Mellon University

Diffusion Models

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Lecture 7
Feb. 5, 2025

Reminders

- **Homework 1: Generative Models of Text**
  - Out: Mon, Jan 27
  - Due: Mon, Feb 10 at 11:59pm
- **Quiz 2:**
  - In-class: Mon, Feb 17
  - Lectures 5-8
- **Homework 2: Generative Models of Images**
  - Out: Mon, Feb 10
  - Due: Sat, Feb 22 at 11:59pm

UNSUPERVISED LEARNING

Unsupervised Learning

Recall…

Assumptions:

1. our data comes from some distribution $p^*(\mathbf{x}_0)$
2. we choose a distribution $p_\theta(\mathbf{x}_0)$ for which sampling $x_0 \sim p_\theta(\mathbf{x}_0)$ is tractable

Goal: learn θ s.t. $p_\theta(\mathbf{x}_0) \approx p^*(\mathbf{x}_0)$

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Goal: learn θ s.t. $p_\theta(\mathbf{x}_0) \approx p^*(\mathbf{x}_0)$

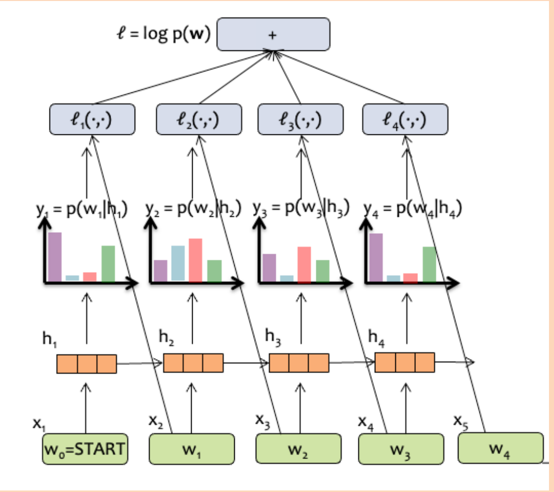
Example: autoregressive LMs

- true $p^*(\mathbf{x}_0)$ is the (human) process that produced text on the web
- choose $p_\theta(\mathbf{x}_0)$ to be an autoregressive language model
  - autoregressive structure means that $p(\mathbf{x}_t \mid \mathbf{x}_1, \ldots, \mathbf{x}_{t-1}) \sim$ Categorical(.) and ancestral sampling is exact/efficient
- learn by finding

  $$\theta \approx \text{argmax}_\theta \log(p_\theta(\mathbf{x}_0))$$

  using gradient based updates on

  $$\nabla_\theta \log(p_\theta(\mathbf{x}_0))$$



Unsupervised Learning

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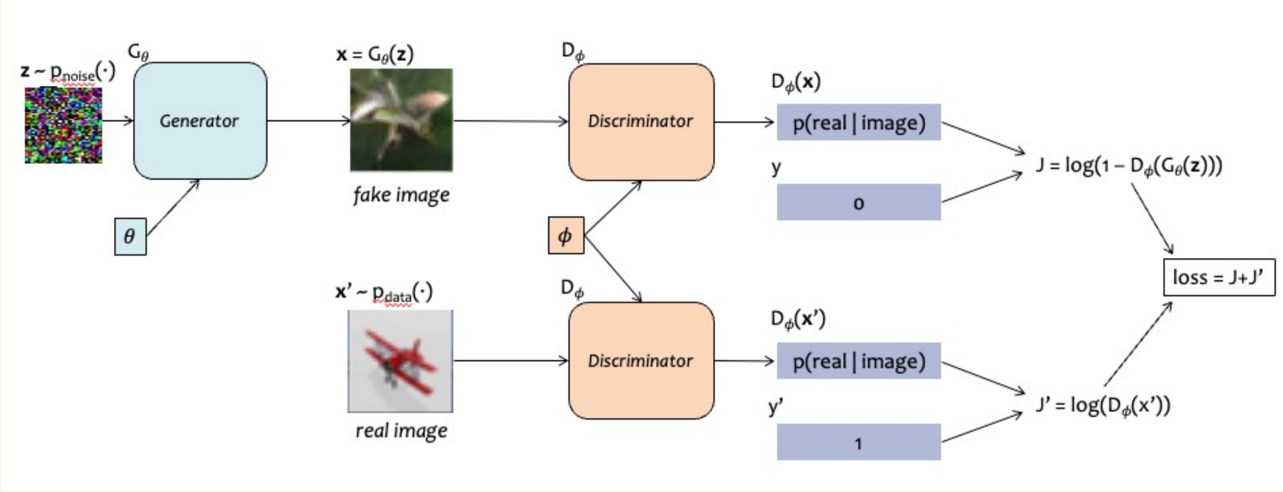
Goal: learn θ s.t. $p_\theta(\mathbf{x}_0) \approx p^*(\mathbf{x}_0)$

Example: GANs

- true $p^*(\mathbf{x}_0)$ is distribution over photos taken and posted to Flikr
- choose $p_\theta(\mathbf{x}_0)$ to be an expressive model (e.g. noise fed into inverted CNN) that can generate images
  - sampling is typically easy: $\mathbf{z} \sim N(\mathbf{0}, \mathbf{I})$ and $\mathbf{x}_0 = f_\theta(\mathbf{z})$
- learn by finding $\theta \approx \text{argmax}_\theta \log(p_\theta(\mathbf{x}_0))$?
  - No! Because we can't even compute $\log(p_\theta(\mathbf{x}_0))$ or its gradient
  - Why not? Because the integral is intractable even for a simple 1-hidden layer neural network with nonlinear activation

$$p(\mathbf{x}_0) = \int_{\mathbf{z}} p(\mathbf{x}_0 \mid \mathbf{z}) p(\mathbf{z}) d\mathbf{z}$$



so optimize a minimax loss instead

Unsupervised Learning

Recall…

Assumptions:

1. our data comes from some distribution $p^*(\mathbf{x}_0)$
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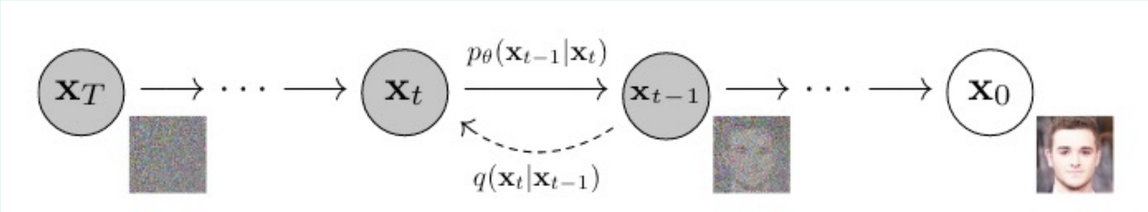


Figure from Ho et al. (2020)

Example: VAEs / Diffusion Models

- true $p^*(\mathbf{x}_0)$ is distribution over photos taken and posted to Flikr
- choose $p_\theta(\mathbf{x}_0)$ to be an expressive model (e.g. noise fed into inverted CNN) that can generate images
  - sampling is will be easy
- learn by finding $\theta \approx \text{argmax}_\theta \log(p_\theta(\mathbf{x}_0))$?
  - Sort of! We can't compute the gradient $\nabla_\theta \log(p_\theta(\mathbf{x}_0))$
  - So we instead optimize a variational lower bound (more on that later)

Latent Variable Models

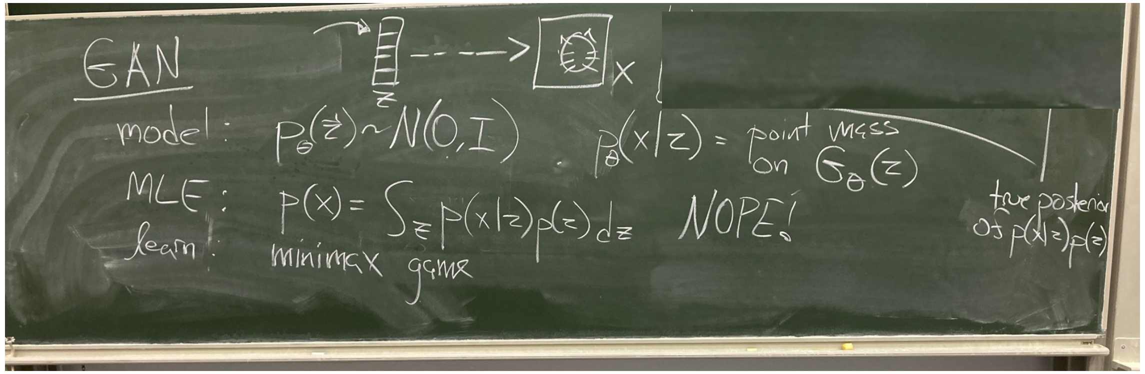
- For GANs and VAEs, we assume that there are (unknown) **latent variables** which give rise to our observations
- The **vector z** are those latent variables
- After learning a GAN or VAE, we can **interpolate** between images in latent **z** space

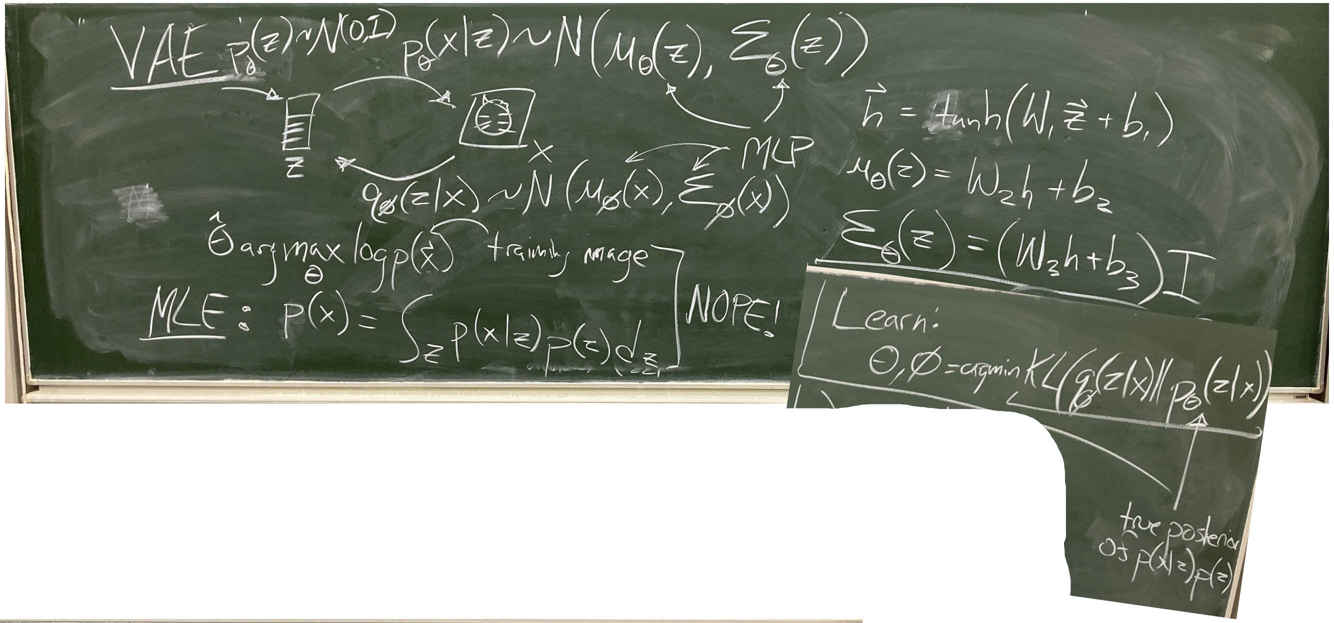
Figure 4: Top rows: Interpolation between a series of 9 random points in Z show that the space learned has smooth transitions, with every image in the space plausibly looking like a bedroom. In the 6th row, you see a room without a window slowly transforming into a room with a giant window. In the 10th row, you see what appears to be a TV slowly being transformed into a window.

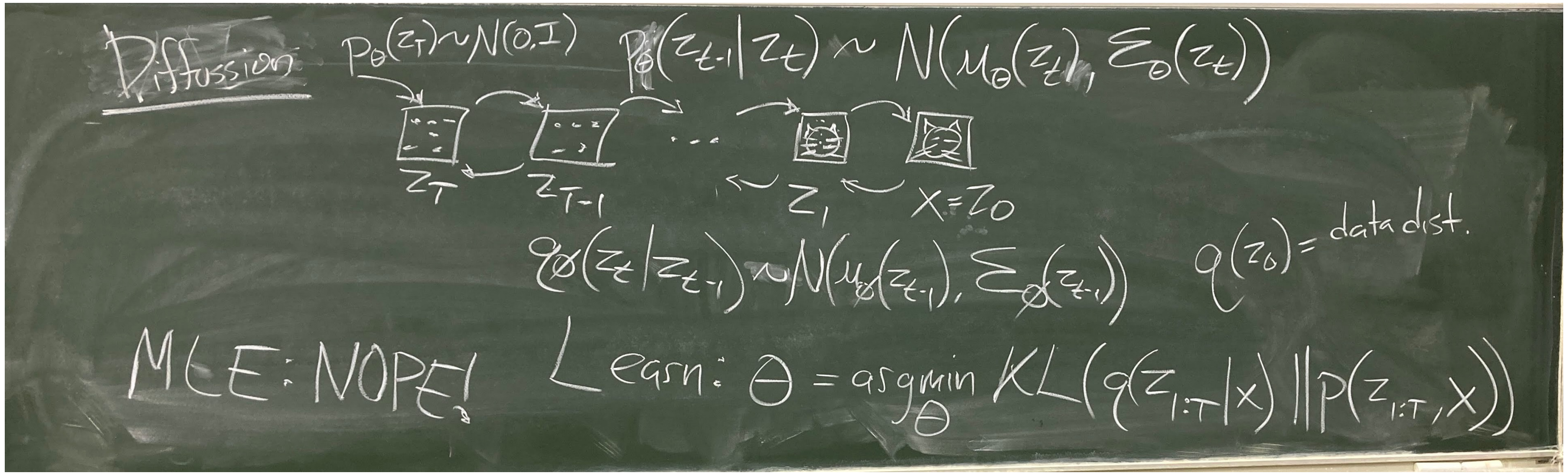
Figure from Radford et al. (2016)

GAN → VAE → Diffusion

(in 15 minutes)



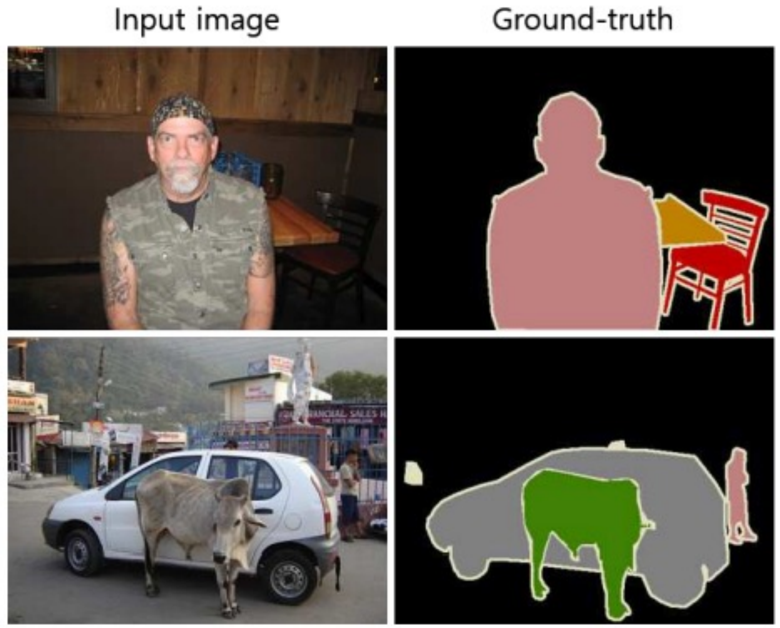




U-NET

Semantic Segmentation

- Given an image, predict a label for every pixel in the image
- Not merely a classification problem, because there are strong correlations between pixel-specific labels



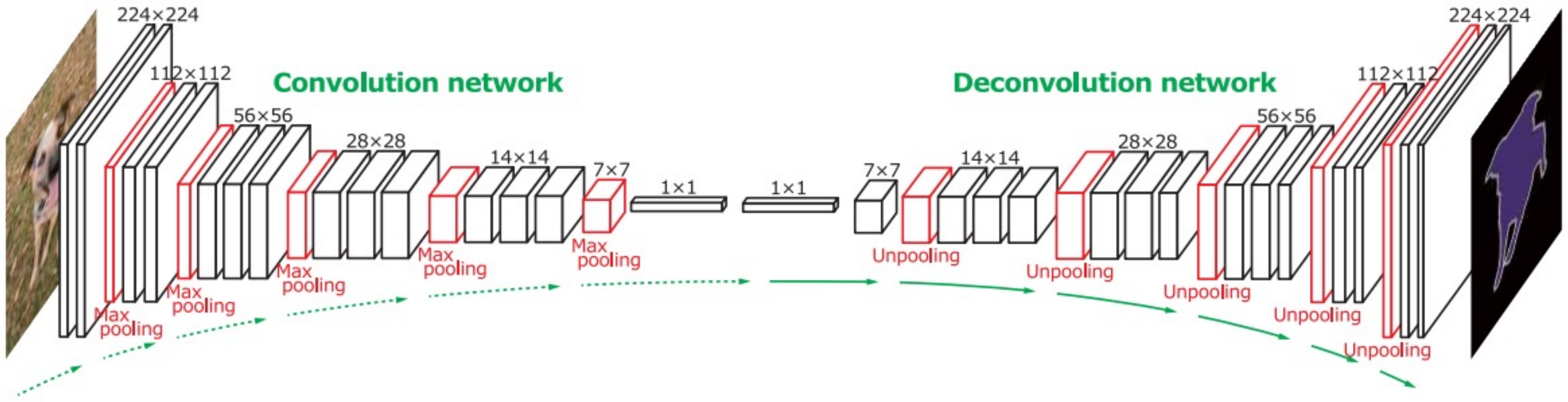


Figure from https://openaccess.thecvf.com/content_iccv_2015/papers/Noh_Learning_Deconvolution_Network_ICCV_2015_paper.pdf

Instance Segmentation

- Predict per-pixel labels as in semantic segmentation, but differentiate between different instances of the same label
- *Example*: if there are two people in the image, one person should be labeled **person-1** and one should be labeled **person-2**

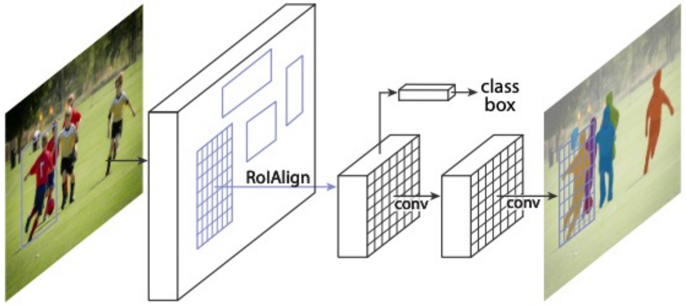
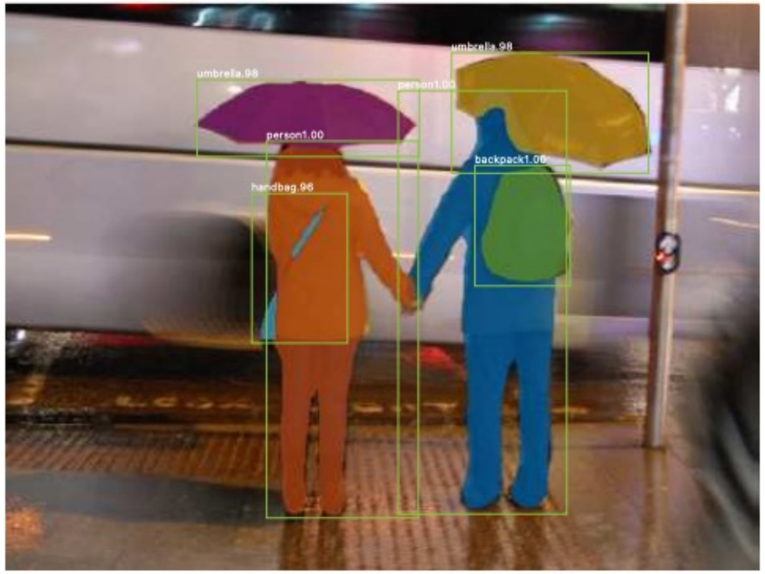


Figure 1. The **Mask R-CNN** framework for instance segmentation.



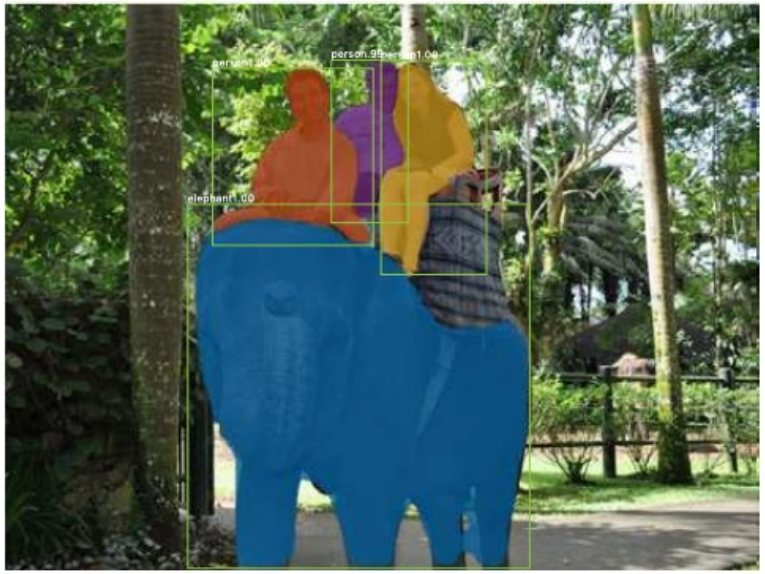


Figure from https://openaccess.thecvf.com/content_ICCV_2017/papers/He_Mask_R-CNN_ICCV_2017_paper.pdf

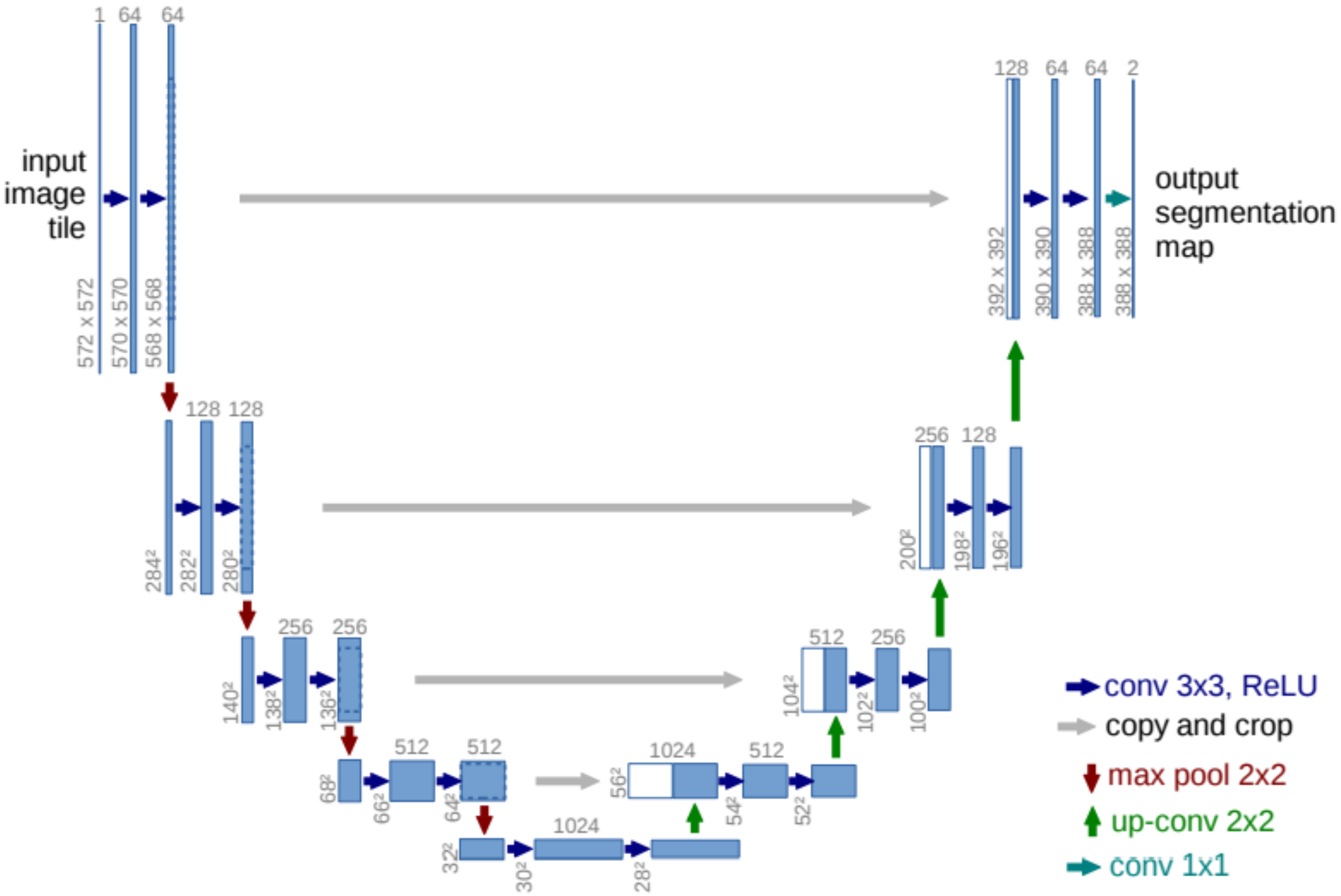
U-Net

Contracting path

- block consists of:
  - 3x3 convolution
  - 3x3 convolution
  - ReLU
  - max-pooling with stride of 2 (downsample)
- repeat the block N times, doubling number of channels

Expanding path

- block consists of:
  - 2x2 convolution (upsampling)
  - concatenation with contracting path features
  - 3x3 convolution
  - 3x3 convolution
  - ReLU
- repeat the block N times, halving the number of channels



U-Net

- Originally designed for applications to biomedical segmentation
- Key observation is that the output layer has the **same** dimensions as the input image (possibly with different number of channels)

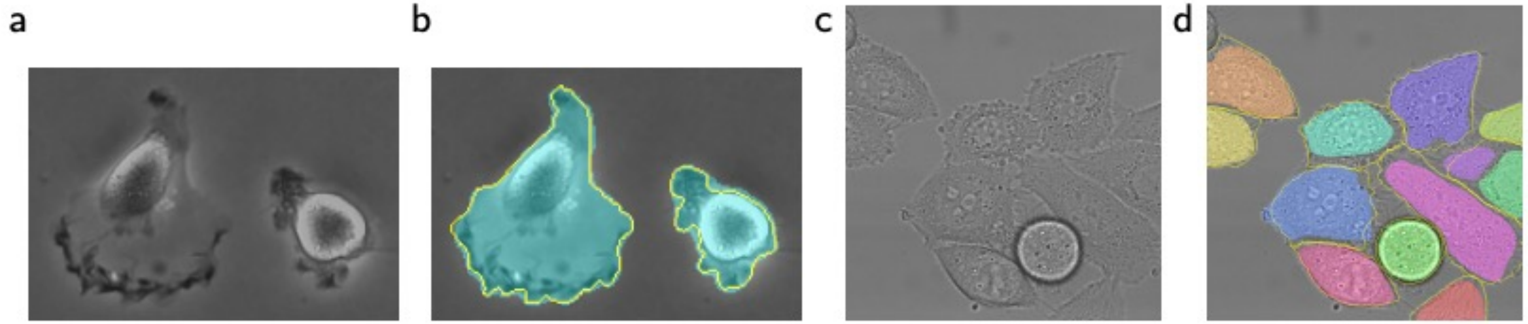
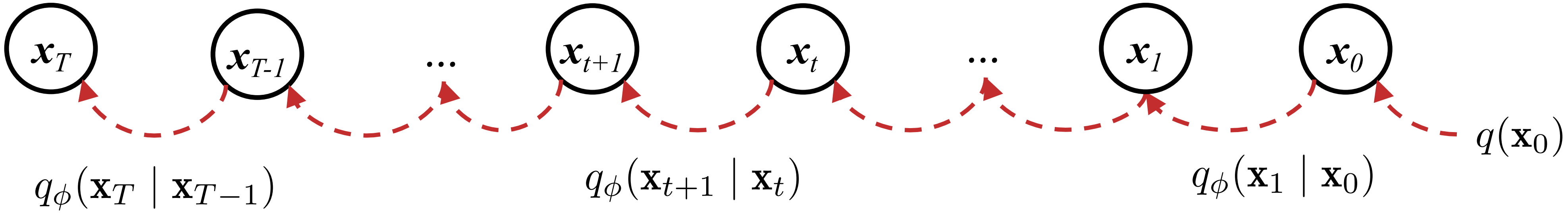


Fig. 4. Result on the ISBI cell tracking challenge. (**a**) part of an input image of the "PhC-U373" data set. (**b**) Segmentation result (cyan mask) with manual ground truth (yellow border) (**c**) input image of the "DIC-HeLa" data set. (**d**) Segmentation result (random colored masks) with manual ground truth (yellow border).

DIFFUSION MODELS

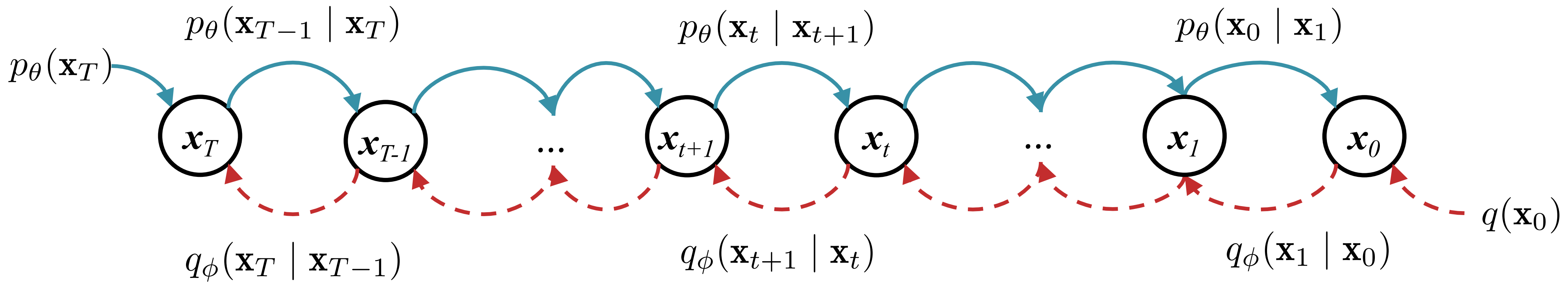
Diffusion Model



Forward Process:

$$q_\phi(\mathbf{x}_{0:T}) = q(\mathbf{x}_0) \prod_{t=1}^{T} q_\phi(\mathbf{x}_t \mid \mathbf{x}_{t-1})$$

Diffusion Model



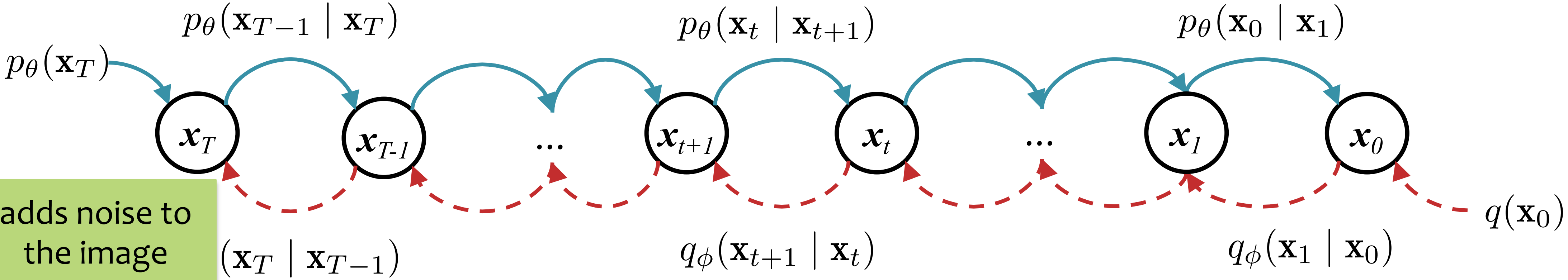
Forward Process:

$$q_\phi(\mathbf{x}_{0:T}) = q(\mathbf{x}_0) \prod_{t=1}^{T} q_\phi(\mathbf{x}_t \mid \mathbf{x}_{t-1})$$

(Learned) Reverse Process:

$$p_\theta(\mathbf{x}_{0:T}) = p_\theta(\mathbf{x}_T) \prod_{t=1}^{T} p_\theta(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$$

Diffusion Model



adds noise to the image

Forward Process:

if we could sample from this we'd be done

$$q_\phi(\mathbf{x}_{0:T}) = q(\mathbf{x}_0) \prod_{t=1}^{T} q_\phi(\mathbf{x}_t \mid \mathbf{x}_{t-1})$$

(Learned) Reverse Process:

removes noise

$$p_\theta(\mathbf{x}_{0:T}) = p_\theta(\mathbf{x}_T) \prod_{t=1}^{T} p_\theta(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$$

goal is to learn this

Diffusion Model

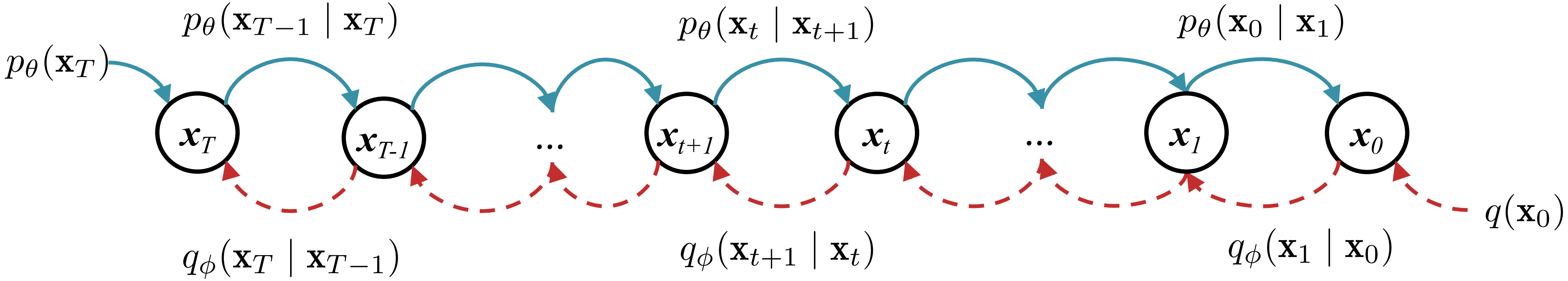
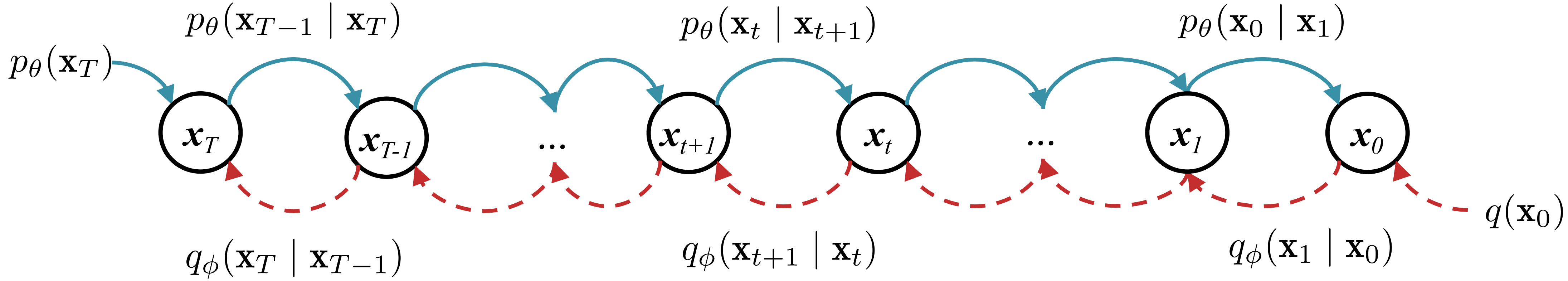
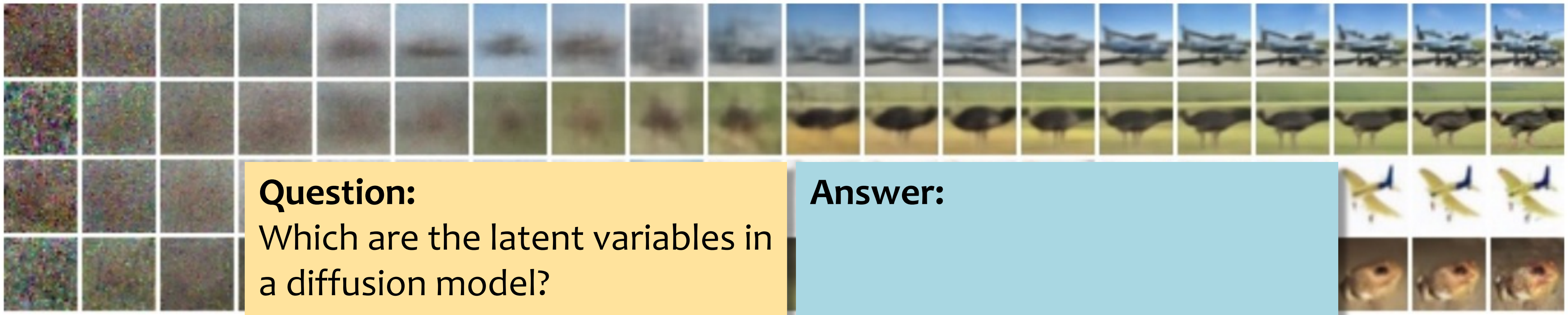


Figure from Ho et al. (2020)

Diffusion Model



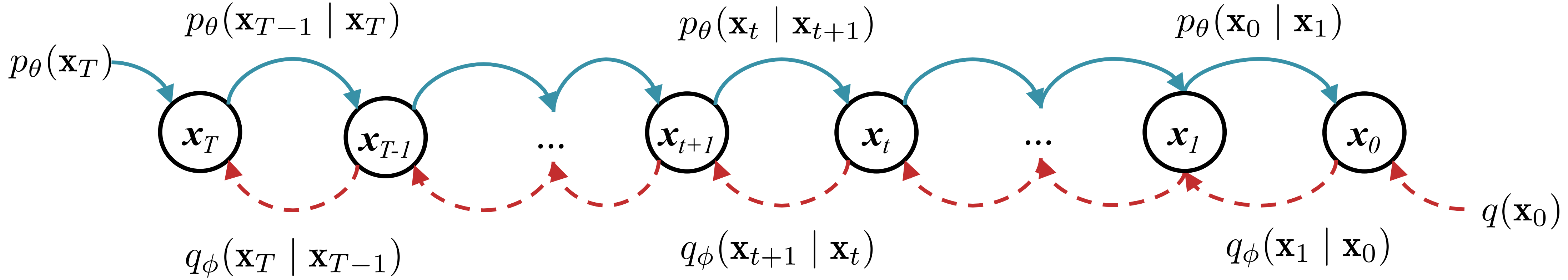


Question:
Which are the latent variables in a diffusion model?

Answer:

Figure from Ho et al. (2020)

Denoising Diffusion Probabilistic Model (DDPM)



Forward Process:

$$q_\phi(\mathbf{x}_{0:T}) = q(\mathbf{x}_0) \prod_{t=1}^{T} q_\phi(\mathbf{x}_t \mid \mathbf{x}_{t-1})$$

$$q(\mathbf{x}_0) = \text{data distribution}$$

$$q_\phi(\mathbf{x}_t \mid \mathbf{x}_{t-1}) \sim \mathcal{N}(\sqrt{\alpha_t}\mathbf{x}_{t-1}, (1-\alpha_t)\mathbf{I})$$

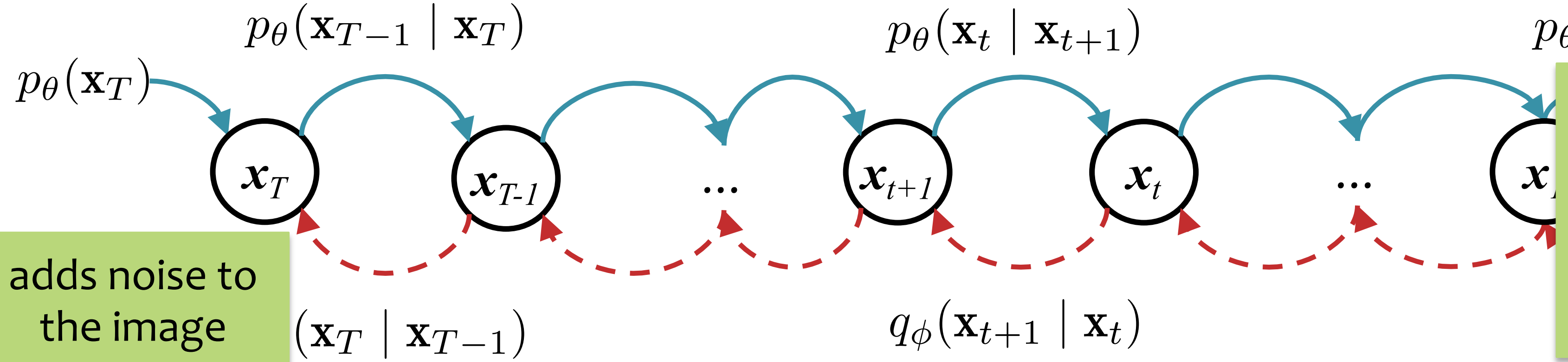
(Learned) Reverse Process:

$$p_\theta(\mathbf{x}_{0:T}) = p_\theta(\mathbf{x}_T) \prod_{t=1}^{T} p_\theta(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$$

$$p_\theta(\mathbf{x}_T) \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

$$p_\theta(\mathbf{x}_{t-1} \mid \mathbf{x}_t) \sim \mathcal{N}(\mu_\theta(\mathbf{x}_t, t), \mathbf{\Sigma}_\theta(\mathbf{x}_t, t))$$

Diffusion Model



learning is hard.
why don't we instead just infer the *exact* reverse process corresponding to the forward process?

adds noise to the image

Forward Process:

if we could sample from this we'd be done

$$q_\phi(\mathbf{x}_{0:T}) = q(\mathbf{x}_0) \prod_{t=1}^{T} q_\phi(\mathbf{x}_t \mid \mathbf{x}_{t-1})$$

(Learned) Reverse Process:

removes noise

$$p_\theta(\mathbf{x}_{0:T}) = p_\theta(\mathbf{x}_T) \prod_{t=1}^{T} p_\theta(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$$

goal is to learn this

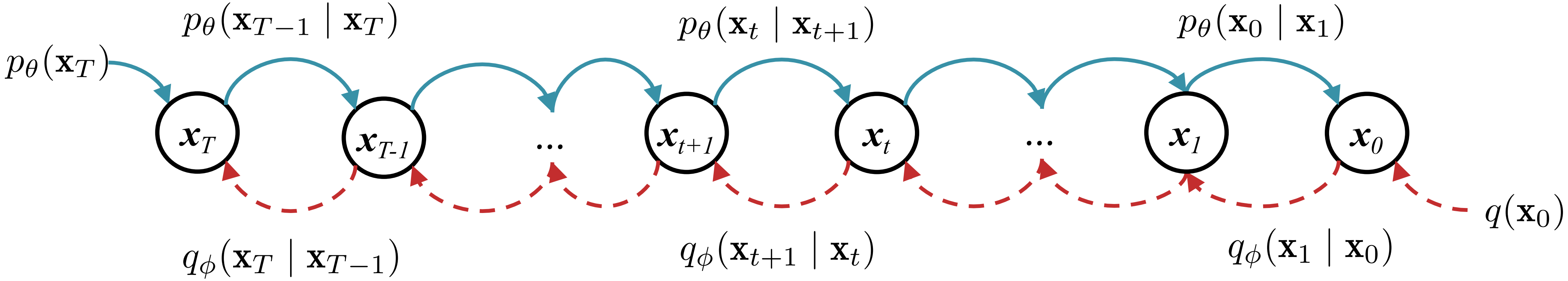
(Exact) Reverse Process:

$$q_\phi(\mathbf{x}_{0:T}) = q_\phi(\mathbf{x}_T) \prod_{t=1}^{T} q_\phi(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$$

The *exact* reverse process requires inference. And, even though $q_\phi(\mathbf{x}_t \mid \mathbf{x}_{t-1})$ is simple, computing $q_\phi(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$ is intractable! Why? Because $q(\mathbf{x}_0)$ might be not-so-simple.

$$q_\phi(\mathbf{x}_{t-1} \mid \mathbf{x}_t) = \frac{\int_{\mathbf{x}_{0:t-2,t+1:T}} q_\phi(\mathbf{x}_{0:T}) d\mathbf{x}_{0:t-2,t+1:T}}{\int_{\mathbf{x}_{0:t-2,t:T}} q_\phi(\mathbf{x}_{0:T}) d\mathbf{x}_{0:t-2,t:T}}$$

Denoising Diffusion Probabilistic Model (DDPM)



Forward Process:

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$$q(\mathbf{x}_0) = \text{data distribution}$$

$$q_\phi(\mathbf{x}_t \mid \mathbf{x}_{t-1}) \sim \mathcal{N}(\sqrt{\alpha_t}\mathbf{x}_{t-1}, (1-\alpha_t)\mathbf{I})$$

(Learned) Reverse Process:

$$p_\theta(\mathbf{x}_{0:T}) = p_\theta(\mathbf{x}_T) \prod_{t=1}^{T} p_\theta(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$$

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Defining the Forward Process

Forward Process:

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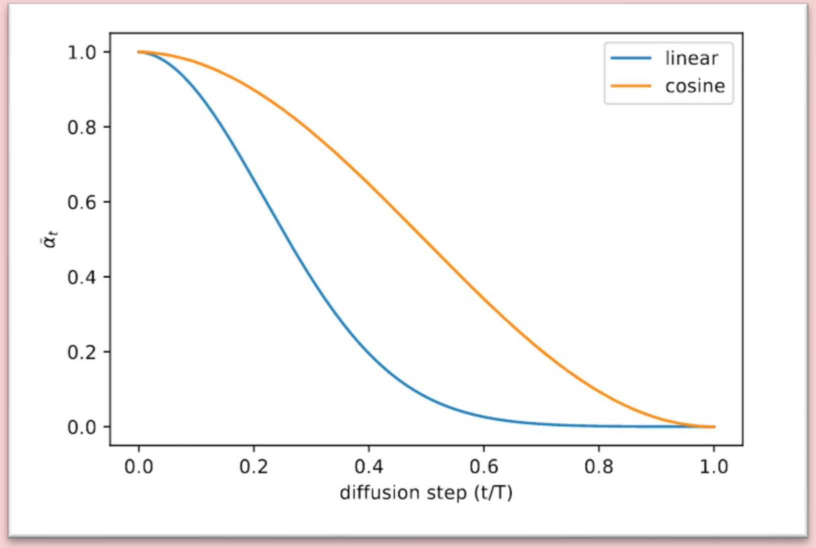
$q(\mathbf{x}_0) =$ data distribution

$$q_\phi(\mathbf{x}_t \mid \mathbf{x}_{t-1}) \sim \mathcal{N}(\sqrt{\alpha_t}\mathbf{x}_{t-1}, (1-\alpha_t)\mathbf{I})$$

Noise schedule:

We choose α_t to follow a fixed schedule s.t. $q_\phi(\mathbf{x}_T) \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$, just like $p_\theta(\mathbf{x}_T)$.



Gaussian (an aside)

Let $X \sim \mathcal{N}(\mu_x, \sigma_x^2)$ and $Y \sim \mathcal{N}(\mu_y, \sigma_y^2)$

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2. Difference of two Gaussians is a Gaussian

$$X - Y \sim \mathcal{N}(\mu_x - \mu_y, \sigma_x^2 + \sigma_y^2)$$

3. Gaussian with a Gaussian mean has a Gaussian Conditional

$$Z \sim \mathcal{N}(\mu_z = X, \sigma_z^2) \Rightarrow P(Z \mid X) \sim \mathcal{N}(\cdot, \cdot)$$

Defining the Forward Process

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$$q_\phi(\mathbf{x}_{0:T}) = q(\mathbf{x}_0) \prod_{t=1}^{T} q_\phi(\mathbf{x}_t \mid \mathbf{x}_{t-1})$$

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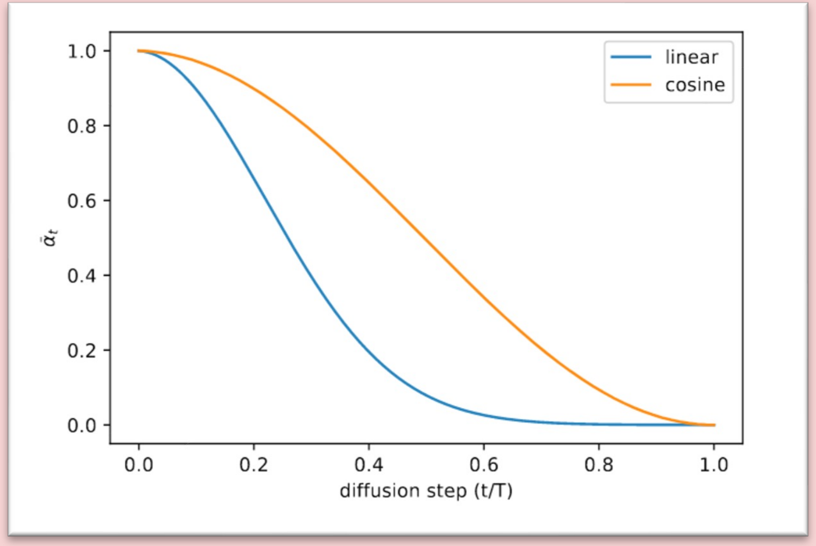


Property #1:

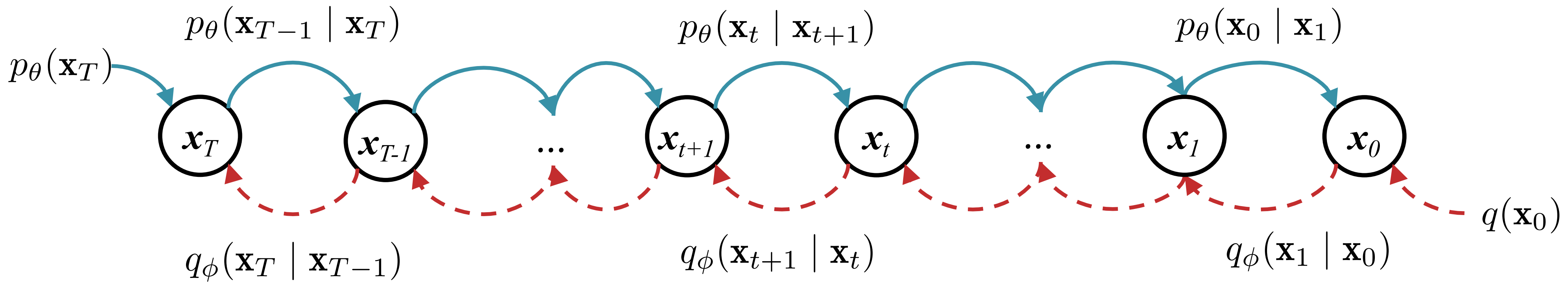
$$q(\mathbf{x}_t \mid \mathbf{x}_0) \sim \mathcal{N}(\sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I})$$

where $\bar{\alpha}_t = \prod_{s=1}^{t} \alpha_s$

Q: So what is $q_\phi(\mathbf{x}_T \mid \mathbf{x}_0)$? Note the *capital* T in the subscript.

A:

Diffusion Model



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Q: If q_ϕ is just adding noise, how can p_θ be interesting at all?

A:

Q: But if $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$ is Gaussian, how can it learn a θ such that $p_\theta(\mathbf{x}_0) \approx q(\mathbf{x}_0)$? Won't $p_\theta(\mathbf{x}_0)$ be Gaussian too?

A:

Gaussian (an aside)

Let $X \sim \mathcal{N}(\mu_x, \sigma_x^2)$ and $Y \sim \mathcal{N}(\mu_y, \sigma_y^2)$

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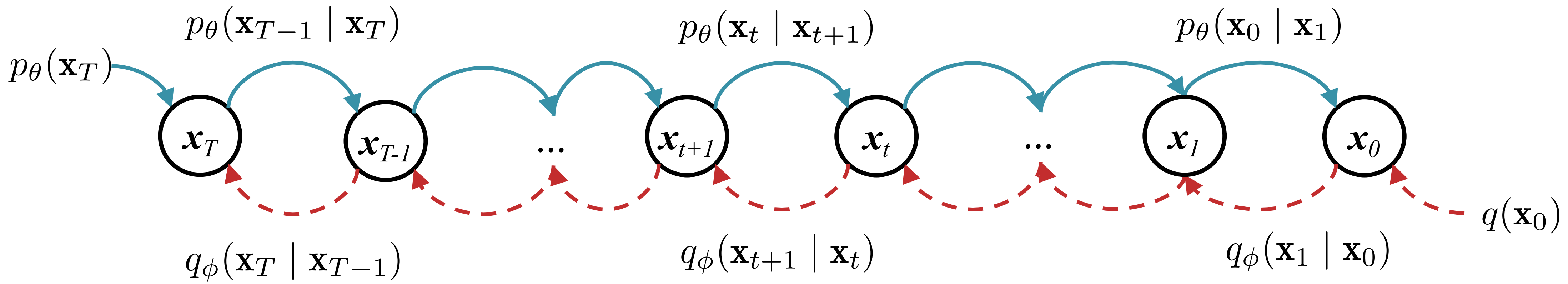
4. But #3 does not hold if X is passed through a nonlinear function f

$$W \sim \mathcal{N}(\mu_z = f(X), \sigma_w^2) \nRightarrow P(W \mid X) \sim \mathcal{N}(\cdot, \cdot)$$

Diffusion Model



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A:

Diffusion Model Analogy

Properties of forward and *exact* reverse processes

Property #1:

$$q(\mathbf{x}_t \mid \mathbf{x}_0) \sim \mathcal{N}(\sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I})$$

where $\bar{\alpha}_t = \prod_{s=1}^{t} \alpha_s$

$\Rightarrow$ we can sample $\mathbf{x}_t$ from $\mathbf{x}_0$ at any timestep t efficiently in closed form

$\Rightarrow$ $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}$ where $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ — this is the same reparameterization trick from VAEs

Properties of forward and *exact* reverse processes

Property #1:

$$q(\mathbf{x}_t \mid \mathbf{x}_0) \sim \mathcal{N}(\sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I})$$

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$\Rightarrow$ we can sample $\mathbf{x}_t$ from $\mathbf{x}_0$ at any timestep t efficiently in closed form

$\Rightarrow$ $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}$ where $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

Property #2: Estimating $q(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$ is intractable because of its dependence on $q(\mathbf{x}_0)$. However, conditioning on $\mathbf{x}_0$ we can efficiently work with:

$$q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\tilde{\mu}_q(\mathbf{x}_t, \mathbf{x}_0), \sigma_t^2\mathbf{I})$$

$$\text{where } \tilde{\mu}_q(\mathbf{x}_t, \mathbf{x}_0) = \frac{\sqrt{\bar{\alpha}_t}(1-\alpha_t)}{1-\bar{\alpha}_t}\mathbf{x}_0 + \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_t)}{1-\bar{\alpha}_t}\mathbf{x}_t$$

$$= \alpha_t^{(0)}\mathbf{x}_0 + \alpha_t^{(t)}\mathbf{x}_t$$

$$\sigma_t^2 = \frac{(1-\bar{\alpha}_{t-1})(1-\alpha_t)}{1-\bar{\alpha}_t}$$

Parameterizing the *learned* reverse process

Recall: $p_\theta(\mathbf{x}_{t-1} \mid \mathbf{x}_t) \sim \mathcal{N}(\mu_\theta(\mathbf{x}_t, t), \mathbf{\Sigma}_\theta(\mathbf{x}_t, t))$

Later we will show that given a training sample $\mathbf{x}_0$, we want

$$p_\theta(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$$

to be as close as possible to

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Intuitively, this makes sense: if the *learned* reverse process is supposed to subtract away the noise, then whenever we're working with a specific $\mathbf{x}_0$ it should subtract it away exactly as *exact* reverse process would have.

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Idea #1: Rather than learn $\Sigma_\theta(\mathbf{x}_t, t)$ just use what we know about $q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0) \sim \mathcal{N}(\tilde{\mu}_q(\mathbf{x}_t, \mathbf{x}_0), \sigma_t^2\mathbf{I})$:

$$\Sigma_\theta(\mathbf{x}_t, t) = \sigma_t^2\mathbf{I}$$

Idea #2: Choose μ_θ based on $q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0)$, i.e. we want $\mu_\theta(\mathbf{x}_t, t)$ to be close to $\tilde{\mu}_q(\mathbf{x}_t, \mathbf{x}_0)$. Here are three ways we could parameterize this:

Option A: Learn a network that approximates $\tilde{\mu}_q(\mathbf{x}_t, \mathbf{x}_0)$ directly from $\mathbf{x}_t$ and t:

$$\mu_\theta(\mathbf{x}_t, t) = \text{UNet}_\theta(\mathbf{x}_t, t)$$

where t is treated as an extra feature in UNet

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$$\mu_\theta(\mathbf{x}_t, t) = \alpha_t^{(0)} \mathbf{x}_\theta^{(0)}(\mathbf{x}_t, t) + \alpha_t^{(t)} \mathbf{x}_t$$

$$\text{where } \mathbf{x}_\theta^{(0)}(\mathbf{x}_t, t) = \text{UNet}_\theta(\mathbf{x}_t, t)$$

Properties of forward and *exact* reverse processes

Property #1:

$$q(\mathbf{x}_t \mid \mathbf{x}_0) \sim \mathcal{N}(\sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I})$$

where $\bar{\alpha}_t = \prod_{s=1}^{t} \alpha_s$

$\Rightarrow$ we can sample $\mathbf{x}_t$ from $\mathbf{x}_0$ at any timestep t efficiently in closed form

$\Rightarrow$ $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}$ where $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

Property #2: Estimating $q(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$ is intractable because of its dependence on $q(\mathbf{x}_0)$. However, conditioning on $\mathbf{x}_0$ we can efficiently work with:

$$q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\tilde{\mu}_q(\mathbf{x}_t, \mathbf{x}_0), \sigma_t^2\mathbf{I})$$

where $\tilde{\mu}_q(\mathbf{x}_t, \mathbf{x}_0) = \frac{\sqrt{\bar{\alpha}_t}(1-\alpha_t)}{1-\bar{\alpha}_t}\mathbf{x}_0 + \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_t)}{1-\bar{\alpha}_t}\mathbf{x}_t$

$$= \alpha_t^{(0)}\mathbf{x}_0 + \alpha_t^{(t)}\mathbf{x}_t$$

$$\sigma_t^2 = \frac{(1-\bar{\alpha}_{t-1})(1-\alpha_t)}{1-\bar{\alpha}_t}$$

Property #3: Combining the two previous properties, we can obtain a different parameterization of $\tilde{\mu}_q$ which has been shown empirically to help in learning p_θ.

Rearranging $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}$ we have that:

$$\mathbf{x}_0 = \left(\mathbf{x}_t - \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}\right) / \sqrt{\bar{\alpha}_t}$$

Substituting this definition of $\mathbf{x}_0$ into property #2's definition of $\tilde{\mu}_q$ gives:

$$\begin{aligned}
\tilde{\mu}_q(\mathbf{x}_t, \mathbf{x}_0) &= \alpha_t^{(0)}\mathbf{x}_0 + \alpha_t^{(t)}\mathbf{x}_t \\
&= \alpha_t^{(0)}\left(\left(\mathbf{x}_t - \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}\right) / \sqrt{\bar{\alpha}_t}\right) + \alpha_t^{(t)}\mathbf{x}_t \\
&= \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{(1-\alpha_t)}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}\right)
\end{aligned}$$

Parameterizing the *learned* reverse process

Recall: $p_\theta(\mathbf{x}_{t-1} \mid \mathbf{x}_t) \sim \mathcal{N}(\mu_\theta(\mathbf{x}_t, t), \mathbf{\Sigma}_\theta(\mathbf{x}_t, t))$

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Idea #2: Choose μ_θ based on $q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0)$, i.e. we want $\mu_\theta(\mathbf{x}_t, t)$ to be close to $\tilde{\mu}_q(\mathbf{x}_t, \mathbf{x}_0)$. Here are three ways we could parameterize this:

Option C: Learn a network that approximates the $\boldsymbol{\epsilon}$ that gave rise to $\mathbf{x}_t$ from $\mathbf{x}_0$ in the forward process from $\mathbf{x}_t$ and t:

$$\mu_\theta(\mathbf{x}_t, t) = \alpha_t^{(0)} \mathbf{x}_\theta^{(0)}(\mathbf{x}_t, t) + \alpha_t^{(t)} \mathbf{x}_t$$

where $\mathbf{x}_\theta^{(0)}(\mathbf{x}_t, t) = \left(\mathbf{x}_t - \sqrt{1-\bar{\alpha}_t}\,\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) / \sqrt{\bar{\alpha}_t}$

where $\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) = \text{UNet}_\theta(\mathbf{x}_t, t)$

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Option C: Learn a network that approximates the ϵ that gave rise to $\mathbf{x}_t$ from $\mathbf{x}_0$ in the forward process from $\mathbf{x}_t$ and t:

$$\mu_\theta(\mathbf{x}_t, t) = \alpha_t^{(0)} \mathbf{x}_\theta^{(0)}(\mathbf{x}_t, t) + \alpha_t^{(t)} \mathbf{x}_t$$

where $\mathbf{x}_\theta^{(0)}(\mathbf{x}_t, t) = \left(\mathbf{x}_t - \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) / \sqrt{\bar{\alpha}_t}$

where $\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) = \text{UNet}_\theta(\mathbf{x}_t, t)$

DIFFUSION MODEL TRAINING

Learning the Reverse Process

Recall: given a training sample $\mathbf{x}_0$, we want

$$p_\theta(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$$

to be as close as possible to

$$q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0)$$

Depending on which of the options for parameterization we pick, we get a different training algorithm.

Option C is the best empirically

Algorithm 1 Training (Option C)

```
initialize θ
for e ∈ {1, ..., E} do
    for x_0 ∈ D do
        t ~ Uniform(1, ..., T)
        ϵ ~ N(0, I)
        x_t ← sqrt(ᾱ_t) x_0 + sqrt(1 − ᾱ_t) ϵ
        ℓ_t(θ) ← ‖ϵ − ϵ_θ(x_t, t)‖²
        θ ← θ − ∇_θ ℓ_t(θ)
```

Option C: Learn a network that approximates the ϵ that gave rise to $\mathbf{x}_t$ from $\mathbf{x}_0$ in the forward process from $\mathbf{x}_t$ and t:

$$\mu_\theta(\mathbf{x}_t, t) = \alpha_t^{(0)} \mathbf{x}_\theta^{(0)}(\mathbf{x}_t, t) + \alpha_t^{(t)} \mathbf{x}_t$$

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